Linear Algebra and its Applications 434 (2011) 1793–1798

Contents lists available at ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

A characterization of graphs with rank 4

Gerard J. Chang [a,b,c,1], Liang-Hao Huang [d,2], Hong-Gwa Yeh [d,*,3]

[a] Department of Mathematics, National Taiwan University, Taipei 10617, Taiwan
[b] Institute for Mathematical Sciences, National Taiwan University, Taipei 10617, Taiwan
[c] National Center for Theoretical Sciences, Taipei Office, Taiwan
[d] Department of Mathematics, National Central University, Jhongli City, Taoyuan 32001, Taiwan

ARTICLE INFO

Article history:
Received 9 November 2009
Accepted 21 September 2010
Available online 12 October 2010

Submitted by R.A. Brualdi

AMS classification:
05C50
15A18
05C75
05C76

Keywords:
Nullity
Rank
Adjacency matrix
Graph
Spectrum

ABSTRACT

The rank of a graph G is defined to be the rank of its adjacency matrix. In this paper, we consider the following problem: What is the structure of a connected graph with rank 4? This question has not yet been fully answered in the literature, and only some partial results are known. In this paper we resolve this question by completely characterizing graphs G whose adjacency matrix has rank 4.

1. Introduction

A *graph* G consists of a finite set $V(G)$ of *vertices* and a finite set $E(G)$ of unordered pairs of vertices called *edges*. A *unicyclic* (resp. *bicyclic*) graph is a connected graph in which the number of edges equals

* Corresponding author.
E-mail addresses: gjchang@math.ntu.edu.tw (G.J. Chang), r90221003@gmail.com (L.-H. Huang), hgyeh@math.ncu.edu.tw (H.-G. Yeh).
1 Partially supported by National Science Council under grant NSC98-2115-M-002-013-MY3.
2 Partially supported by National Science Council under grant NSC99-2811-M-008-059.
3 Partially supported by National Science Council under grant NSC97-2628-M-008-018-MY3.

0024-3795/$ - see front matter © 2010 Elsevier Inc. All rights reserved.
doi:10.1016/j.laa.2010.09.040

the number of vertices (resp. plus one). Throughout this paper, we consider finite graphs with no loops or multiple edges, and use the notation and terminology of [2], unless otherwise stated.

The *adjacency matrix* $A(G)$ of a graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$ is the $n \times n$ symmetric matrix $[a_{ij}]$ such that $a_{ij} = 1$ if v_i is adjacent to v_j, and $a_{ij} = 0$ otherwise. The *rank* of a graph G, written as $r(G)$, is defined to be the rank of its adjacency matrix $A(G)$ (or, equivalently, the number of nonzero eigenvalues of $A(G)$). We will say that G has rank k if $r(G) = k$. The *nullity* of a graph G is the nullity of its adjacency matrix $A(G)$ (or, equivalently, the multiplicity of the zero eigenvalues of $A(G)$) and is denoted by $\eta(G)$. We will say that G has nullity t if $\eta(G) = t$. Clearly, we have $\eta(G) = |V(G)| - r(G)$. If $\eta(G) \geqslant 1$, then G is said to be *singular*.

In chemistry, a conjugated hydrocarbon molecule can be modeled by its molecular graph G, where the vertices of G represent the carbon atoms, and the edges of G represent the carbon–carbon bonds of the conjugated molecule. The nullity (rank) of a molecular graph G has a number of important applications in chemistry [5–7,23,26,29]. For example, it was known that $\eta(G) = 0$ is a necessary condition for the molecule represented by G to be chemically stable [8,9,12].

In 1957, Collatz and Sinogowitz [5] posed the problem of characterizing all singular graphs. The problem is very hard; only some particular results are known [3,9,10,14,15,19,21,22,24,25,28,30]. Motivated by the problem of determining the structural features that force a graph G to be singular, many papers investigated the influence of $\eta(G)$ (or, equivalently, $r(G)$) on the structure of the graph G and vice versa (see [1,15,16,17,20] for examples).

It was shown in [23] (see also [4,16]) that graphs G with $r(G)$ equal to 2 or 3 can be completely characterized. A natural question to ask next is: What is the structure of a graph G with rank $r(G) = 4$?

This question has not yet been fully answered in the literature, and only some partial results are known: A characterization of bicyclic graph G with rank $r(G) = 4$ was given by Hu et al. [16]; A characterization of connected graph G having pendant vertices with rank $r(G) = 4$ was shown in [18]; In [11], Fan and Qian characterized bipartite graphs G with rank $r(G) = 4$; Tan and Liu [27] (see also [14]) characterized unicyclic graphs G with $r(G) = 4$.

In Theorem 2 of this paper we completely characterize the structure of a connected graph with rank 4. This completely answers the question posed above.

2. Main result

In this section we prove our main result, that is we determine those connected graphs G with $r(G) = 4$. Before proving Theorem 2, we need some notation and a proposition.

For a vertex x in G, the set of all vertices in G that are adjacent to x is denoted by $N_G(x)$. An edge $\{u, v\}$ between vertices u and v of G is also denoted by uv. The *distance* between u and v, denoted by $\mathrm{dist}_G(u, v)$, is the length of a shortest u, v-path in graph G. The distance between a vertex u and a subgraph H of G, denoted by $\mathrm{dist}_G(u, H)$, is defined to be the value $\min\{\mathrm{dist}_G(u, v) : v \in V(H)\}$. Given a subset $S \subseteq V(G)$, the *subgraph (of G) induced by S*, written as $G[S]$, is defined to be the graph with vertex set S and edge set $\{xy \in E(G) : x \in S \text{ and } y \in S\}$. If $S = \{u_1, u_2, \ldots, u_t\}$, for brevity, we denote by $G[u_1, u_2, \ldots, u_t]$ the graph $G[S]$.

A subset $I \subseteq V(G)$ is called an *independent set* of G if there are no edges between any two vertices in I. The *n-path* is the graph P_n with $V(P_n) = \{v_1, v_2, \ldots, v_n\}$ and $E(P_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n\}$. The *n-cycle* is the graph C_n with $V(C_n) = \{v_1, v_2, \ldots, v_n\}$ and $E(C_n) = \{v_1v_2, v_2v_3, \ldots, v_{n-1}v_n, v_nv_1\}$. The *complete graph* on n vertices has n vertices and $n(n-1)/2$ edges, and is denoted by K_n.

Next we define a well-known graph operation called multiplication of vertices (see page 53 of [13]). Given a graph G with $V(G) = \{v_1, v_2, \ldots, v_n\}$. Let

$$\mathbf{m} = (m_1, m_2, \ldots, m_n)$$

be a vector of positive integers. Denote by $G \circ \mathbf{m}$ the graph obtained from G by replacing each vertex v_i of G with an independent set of m_i vertices $v_i^1, v_i^2, \ldots, v_i^{m_i}$ and joining v_i^s with v_j^t if and only if v_i and v_j are adjacent in G. The resulting graph $G \circ \mathbf{m}$ is said to be obtained from G by *multiplication of vertices*. For graphs $G_1, G_2, \ldots, G_k$, we denote by $\mathcal{M}(G_1, G_2, \ldots, G_k)$ the class of all graphs that can be obtained from one of the graphs in $\{G_1, G_2, \ldots, G_k\}$ by multiplication of vertices. As examples, in Fig. 1, it can be seen that $\{Q_1, Q_6\} \subseteq \mathcal{M}(P_4)$, $\{Q_2, Q_3\} \subseteq \mathcal{M}(P_5)$, $Q_4 \in \mathcal{M}(C_5)$ and $Q_5 \in \mathcal{M}(K_3)$.

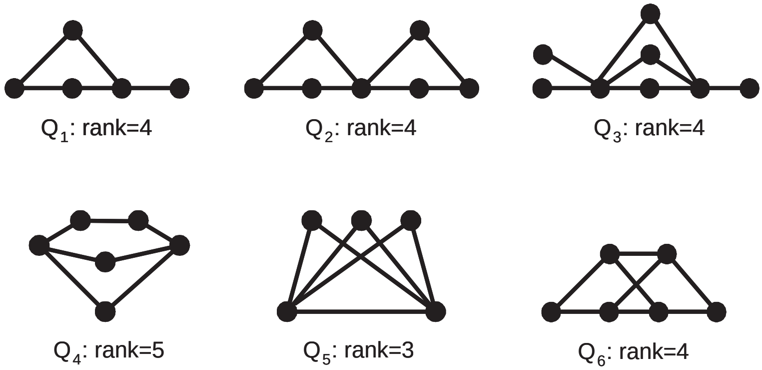

Fig. 1. The graphs $Q_1, Q_2, Q_3, Q_4, Q_5, Q_6$ and their ranks.

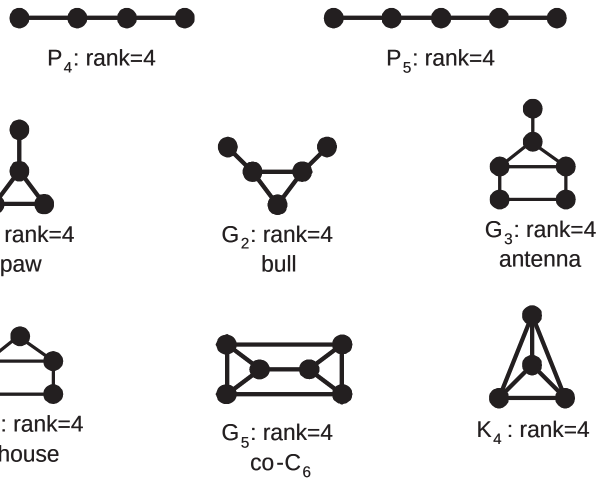

Fig. 2. The graphs $G_1, G_2, G_3, G_4, G_5, P_4, P_5, K_4$ and their ranks.

The following proposition is implicitly used throughout the proof of Theorem 2. The proof of Proposition 1 is straightforward and hence omitted.

Proposition 1. *Suppose that G and H are two graphs. If $G \in \mathcal{M}(H)$, then $r(G) = r(H)$.*

Theorem 2. *Let G be a connected graph. Then $r(G) = 4$ if and only if G can be obtained from one of the graphs shown in Fig. 2 by multiplication of vertices.*

Proof. The sufficient part is clear. We now prove the necessary part. Assume that $r(G) = 4$. For brevity of notation, we denote by $\mathcal{F}$ the set

$$\mathcal{M}(G_1, G_2, G_3, G_4, G_5, P_4, P_5, K_4).$$

By Theorem 3.2 of [11], we see that if G is bipartite, then $G \in \mathcal{M}(P_4, P_5)$ and hence $G \in \mathcal{F}$.

Thus, we may assume that G is not bipartite. Let C_{2k+1} be the smallest odd cycle in G. We claim that $k = 1$. Indeed, if $k \geqslant 2$, then G contains either C_5 or P_6 as an induced subgraph. But this contradicts to our assumption that $r(G) = 4$, since $r(C_5) = 5$ and $r(P_6) = 6$.

Now suppose that C is a 3-cycle in G with vertex set $V(C) = \{a, b, c\}$. We claim that $\mathrm{dist}_G(x, C) \leqslant 1$ for every vertex x of G. If not, there would exist a vertex v in G such that $\mathrm{dist}_G(v, C) = 2$. It follows that G

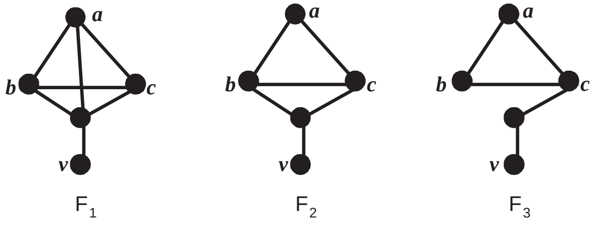

Fig. 3. The graphs $F_1,\ F_2,\ F_3$.

contains an induced subgraph isomorphic to one of the graphs depicted in Fig. 3. This is a contradiction, however, since each graph in Fig. 3 has rank 5.

Let $\overline{C}$ be the subgraph of G induced by the vertices of G not in C. For a vertex subset U of C, denote by S_U the set $\{x \in V(\overline{C}) : N_G(x) \cap V(C) = U\}$. The key ingredients of the remaining proof are the following six claims, which together imply that $G \in \mathcal{F}$.

Claim 1. *$S_{\{a\}}, S_{\{a,b\}}$ and $S_{\{a,b,c\}}$ are independent sets in G.*

Claim 2. *Either $S_{\{a\}} \bigcup S_{\{b\}} \bigcup S_{\{c\}}$ or $S_{\{a,b,c\}}$ is an empty set.*

Claim 3. *Suppose that $y \in S_{\{a,b\}}$. (a) If $x \in S_{\{a\}}$, then x is not adjacent to y. (b) If $x \in S_{\{c\}}$, then x is adjacent to y.*

Claim 4. *Suppose that $y \in S_{\{a,b\}}$. (a) If $x \in S_{\{a,c\}}$, then x is adjacent to y. (b) If $x \in S_{\{a,b,c\}}$, then x is adjacent to y.*

Claim 5. *Suppose that $\{x, y\} \subseteq S_{\{a\}}$ and $z \in S_{\{b\}}$. If x is adjacent to z, then y is adjacent to z.*

Claim 6. *Suppose that $x \in S_{\{a\}},\ y \in S_{\{b\}}$ and $z \in S_{\{c\}}$. If x is adjacent to both y and z, then y is adjacent to z.*

We now prove the above claims in order:

Proof of Claim 1. Assume, to the contrary, that $S_{\{a\}}, S_{\{a,b\}}$ and $S_{\{a,b,c\}}$ are not independent sets of G. If there are two vertices x, y in $S_{\{a\}}$ such that x is adjacent to y, then $G[a, b, c, x, y]$ is isomorphic to the graph H_1 shown in Fig. 4, and hence $r(G) \geqslant r(H_1) = 5$, a contradiction. If there are two vertices x, y in $S_{\{a,b\}}$ such that x is adjacent to y, then $G[a, b, c, x, y]$ is isomorphic to the graph H_2 shown in Fig. 4, and hence $r(G) \geqslant r(H_2) = 5$, a contradiction. Finally, if there are two vertices x, y in $S_{\{a,b,c\}}$ such that x is adjacent to y, then $G[a, b, c, x, y]$ is a complete graph on 5 vertices, and hence $r(G) \geqslant r(K_5) = 5$, a contradiction. □

Proof of Claim 2. Assume, to the contrary, that there exist vertices $x,\ y$ such that $x \in S_{\{a\}}$ and $y \in S_{\{a,b,c\}}$. It follows that $G[a, b, c, x, y]$ is isomorphic to either the graph H_2 shown in Fig. 4 or the graph F_1 shown in Fig. 3, and hence $r(G) \geqslant 5$, a contradiction. □

Proof of Claim 3. (a) Assume, to the contrary, that x is adjacent to y. It follows that $G[a, b, c, x, y]$ is isomorphic to the graph H_3 shown in Fig. 4, and hence $r(G) \geqslant r(H_3) = 5$, a contradiction.

(b) Assume, to the contrary, that x is not adjacent to y. It can be seen that $G[a, b, c, x, y]$ is isomorphic to the graph F_2 shown in Fig. 3, and hence $r(G) \geqslant r(F_2) = 5$, a contradiction. □

Proof of Claim 4. (a) Assume, to the contrary, that x is not adjacent to y. It follows that $G[a, b, c, x, y]$ is isomorphic to the graph H_3 shown in Fig. 4, and hence $r(G) \geqslant r(H_3) = 5$, a contradiction. Therefore x must be adjacent to y.

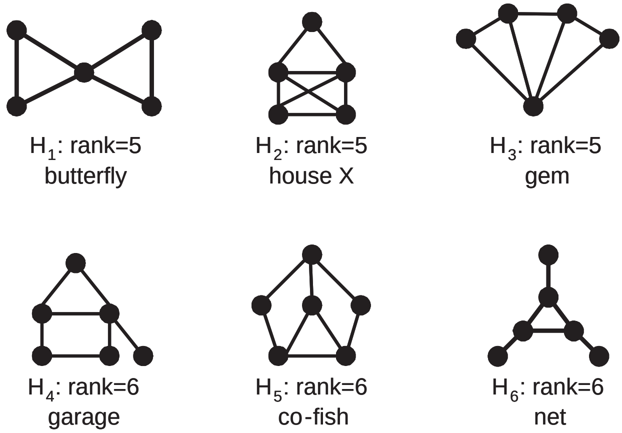

Fig. 4. The graphs $H_1, H_2, H_3, H_4, H_5, H_6$ and their ranks.

(b) Assume, to the contrary, that x is not adjacent to y. It can be seen that $G[a, b, c, x, y]$ is isomorphic to the graph H_2 shown in Fig. 4, and hence $r(G) \geqslant r(H_2) = 5$, a contradiction. Therefore x must be adjacent to y. $\square$

Proof of Claim 5. To verify this claim first note that, by Claim 1, y is not adjacent to x. Now assume that y is also not adjacent to z. It can be seen that $G[a, b, c, x, y, z]$ is isomorphic to the graph H_4 shown in Fig. 4, and hence $r(G) \geqslant r(H_4) = 6$, a contradiction. Therefore y must be adjacent to z. $\square$

Proof of Claim 6. Assume, to the contrary, that y is not adjacent to z. It turns out that $G[a, b, c, x, y, z]$ is isomorphic to the graph H_5 shown in Fig. 4, and hence $r(G) \geqslant r(H_5) = 6$, a contradiction. Therefore y must be adjacent to z. $\square$

We are now in a position to complete the proof of Theorem 2. We divide the remaining proof into two cases based on the set $S_{\{a,b,c\}}$. First, we introduce a notation that will be used later. Denote by S_2 the set $S_{\{a,b\}} \bigcup S_{\{b,c\}} \bigcup S_{\{c,a\}}$.

Case 1. $S_{\{a,b,c\}}$ is not an empty set. In this case, by Claim 2, $S_{\{a\}}, S_{\{b\}}, S_{\{c\}}$ are empty sets, and hence $G = G[V(C) \bigcup S_2 \bigcup S_{\{a,b,c\}}]$. Note that Claim 1 implies that $G[V(C) \bigcup S_{\{a,b,c\}}] \in \mathcal{M}(K_4)$, and Claim 4(a) together with Claim 1 imply that $G[V(C) \bigcup S_2] \in \mathcal{M}(K_3)$. With the aid of Claim 4(b) we conclude that $G[V(C) \bigcup S_2 \bigcup S_{\{a,b,c\}}] \in \mathcal{M}(K_4)$, and hence $G \in \mathcal{M}(K_4) \subseteq \mathcal{F}$.

Case 2. $S_{\{a,b,c\}}$ is an empty set. In this case, clearly $S_{\{a\}} \bigcup S_{\{b\}} \bigcup S_{\{c\}}$ is not an empty set, since otherwise, by Claims 1 and 4(a), $G = G[V(C) \bigcup S_2] \in \mathcal{M}(K_3)$, contradicting to our assumption that $r(G) = 4$. In the following, we want to show that

$$G \in \mathcal{M}(G_1, G_2, G_3, G_4, G_5),$$

and hence $G \in \mathcal{F}$. Towards this end, due to symmetry, only the following three scenarios need to be considered:

1. $S_{\{a\}}$ is not empty, while $S_{\{b\}}$ and $S_{\{c\}}$ are empty.
2. $S_{\{a\}}$ and $S_{\{b\}}$ are not empty, while $S_{\{c\}}$ is empty.
3. $S_{\{a\}}, S_{\{b\}}$ and $S_{\{c\}}$ are not empty.

In Scenario 1, by Claims 4(a), 3 and 1, it is easy to check that $G = G[V(C) \cup S_2 \cup S_{\{a\}}] \in \mathcal{M}(G_1)$, where G_1 is shown in Fig. 2.

In Scenario 2, by Claim 5 and what we have proved in Scenario 1 above, it can be seen that $G = G[V(C) \bigcup S_2 \bigcup S_{\{a\}} \bigcup S_{\{b\}}] \in \mathcal{M}(G_2, G_4)$, where G_2, G_4 are shown in Fig. 2.

In Scenario 3, by Claim 6 and what we have proved in Scenario 2 above, it can be seen that $G = G[V(C) \bigcup S_2 \bigcup S_{\{a\}} \bigcup S_{\{b\}} \bigcup S_{\{c\}}] \in \mathcal{M}(G_3, G_5, H_6)$, where G_3, G_5 are shown in Fig. 2 and H_6 is shown in Fig. 4. Since $r(H_6) = 6$, it must be that $G \notin \mathcal{M}(H_6)$. Therefore, we have $G \in \mathcal{M}(G_3, G_5)$.

What we have proved so far can be summed up by saying that

$$G \in \mathcal{M}(G_1, G_2, G_3, G_4, G_5, P_4, P_5, K_4).$$

This completes the proof of Theorem 2. □

Acknowledgments

The authors would like to thank the anonymous referee for very careful reading and for helpful comments which helped to improve the presentation of the paper.

References

[1] F. Ashraf, H. Bamdad, A note on graphs with zero nullity, Match 60 (2008) 15–19.
[2] J.A. Bondy, U.S.R. Murty, Graph Theory, Graduate Texts in Mathematics, vol. 244, Springer-Verlag, New York, 2008.
[3] M. Brown, J.W. Kennedy, B. Servatius, Graph singularity, Graph Theory Notes N. Y. 25 (1993) 23–32.
[4] B. Cheng, B. Liu, On the nullity of graphs, Electron. J. Linear Algebra 16 (2007) 60–67.
[5] L. Collatz, U. Sinogowitz, Spektren endlicher Grafen, Abh. Math. Sem. Univ. Hamburg 21 (1957) 63–77.
[6] F.A. Cotton, Chemical Applications of Group Theory, InterScience, New York, 1963., pp. 117–182.
[7] D. Cvetković, I. Gutman, The algebraic multiplicity of the number zero in the spectrum of a bipartite graph, Mat. Vesnik 9 (1972) 141–150.
[8] D. Cvetković, I. Gutman, N. Trinajstić, Graphical studies on the relations between the structure and reactivity of conjugated system: the role of non-bonding molecular orbitals, J. Mol. Struct. 28 (1975) 289–303.
[9] D. Cvetković, M. Doob, H. Sachs, Spectra of Graphs – Theory and Application, Academic Press, New York, 1980.
[10] S. Fiorini, I. Gutman, I. Sciriha, Trees with maximum nullity, Linear Algebra Appl. 397 (2005) 245–251.
[11] Y.-Z. Fan, K.-S. Qian, On the nullity of bipartite graphs, Linear Algebra Appl. 430 (2009) 2943–2949.
[12] A. Graovac, I. Gutman, N. Trinajstić, Topological Approach to the Chemistry of Conjugated Molecules, Springer, Berlin, 1977.
[13] M.C. Golumbic, Algorithmic Graph Theory and Perfect Graphs, Academic Press, New York, 1980.
[14] J.-M. Guo, W. Yan, Y.-N. Yeh, On the nullity and the matching number of unicyclic graphs, Linear Algebra Appl. 431 (2009) 1293–1301.
[15] I. Gutman, I. Sciriha, On the nullity of line graphs of trees, Discrete Math. 232 (2001) 35–45.
[16] S. Hu, X. Tan, Bolian Liu, On the nullity of bicyclic graphs, Linear Algebra Appl. 429 (2008) 1387–1391.
[17] W. Li, A. Chang, On the trees with maximum nullity, Match 56 (2006) 501–508.
[18] S. Li, On the nullity of graphs with pendent vertices, Linear Algebra Appl. 429 (2008) 1619–1628.
[19] M. Nath, B.K. Sarma, On the null-spaces of acyclic and unicyclic singular graphs, Linear Algebra Appl. 427 (2007) 42–54.
[20] G.R. Omidi, On the nullity of bipartite graphs, Graphs Combin. 25 (2009) 111–114.
[21] I. Sciriha, On the construction of graphs of nullity one, Discrete Math. 181 (1998) 193–211.
[22] I. Sciriha, On singular line graphs of trees, Congr. Numer. 135 (1998) 73–91.
[23] I. Sciriha, On the rank of graphs, in: Y. Alavi, D.R. Lick, A. Schwenk, Combinatorics, Graph Theory, and Algorithms, vol. II, New Issue Press, Western Michigan University, Kalamazoo, Michigan, 1999, pp. 769–778.
[24] I. Sciriha, A characterization of singular graphs, Electron. J. Linear Algebra 16 (2007) 451–462.
[25] I. Sciriha, P.W. Fowler, On nut and core singular fullerenes, Discrete Math. 308 (2008) 267–276.
[26] S. Severini, Two-colorable graph states with maximal Schmidt measure, Phys. Lett. A 356 (2006) 99–103.
[27] X. Tang, B. Liu, On the nullity of unicyclic graphs, Linear Algebra Appl. 408 (2005) 212–220.
[28] R. Wilson, Singular graphs, in: V.R. Kulli (Ed.), Recent Studies in Graph Theory, Vishwa Int. Publications, Gulbarga, 1989, pp. 228–236.
[29] T. Zivković, Calculations of the non-bonding molecular orbitals in the Hükel theory, Croatica Chem. Acta 44 (1972) 351–364.
[30] Y.N. Yeh, I. Gutman, C.M. Fu, Graph transformations which preserve the multiplicity of an eigenvalue, Discrete Appl. Math. 67 (1996) 221–228.